

Partitioned quantum cellular automata are intrinsically universal

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Abstract. There have been several non-axiomatic approaches taken to define Quantum Cellular Automata (QCA). Partitioned QCA (PQCA) are the most canonical of these non-axiomatic definitions. In this work we show that any QCA can be put into the form of a PQCA. Our construction reconciles all the non-axiomatic definitions of QCA, showing that they can all simulate one another, and hence that they are all equivalent to the axiomatic definition. This is achieved by defining generalised n -dimensional intrinsic simulation, which brings the computer science based concepts of simulation and universality closer to theoretical physics. The result is not only an important simplification of the QCA model, it also plays a key role in the identification of a minimal n -dimensional intrinsically universal QCA.

1 Introduction

1.1 QCA: Importance and Competing Definitions

Cellular automata (CA), first introduced by von Neumann [39], consist of an array of identical cells, each of which may take one of a finite number of possible states. The whole array evolves in discrete time steps by iterating a function G . This global evolution G is shift-invariant (it acts in the same way everywhere) and local (information cannot be transmitted faster than some fixed number of cells per time step). Because this is a physics-like model of computation [21], Feynman [15], and later Margolus [22], suggested that quantising this model was important, for two reasons: firstly, because in CA computation occurs without extraneous (unnecessary) control, hence eliminating a source of decoherence; and secondly, because they are a good framework in which to study the quantum simulation of a quantum system. From a computation perspective there are other reasons to study QCA, such as studying space-sensitive problems in computer science (*e.g.* ‘machine self-reproduction’ [39, 23]) in the quantum setting. There is also a theoretical physics perspective, where CA are used as toy models of quantum space-time [20].

These motivations demonstrate the importance of studying QCA. Once this is acknowledged researchers are faced with an overabundance of competing definitions of QCA. An examination shows that there are four main approaches to defining QCA: the axiomatic style [5, 6, 33], the multilayer block representation [5, 31], the two-layer block representation [9, 18, 28, 32, 33, 37], and Partitioned QCA (PQCA) [17, 37, 41]. A natural first question to consider is whether they are equivalent, and in what sense.

1.2 QCA: Simulation and Equivalence

Probably the most well known CA is Conway’s ‘Game of Life’; a two-dimensional CA which has been shown to be universal for computation in the sense that any Turing Machine (TM) can be encoded within its initial state and then executed by evolution of the CA [8]. As TMs are generally considered to be a robust definition of ‘what an algorithm is’ in classical computer science, this result could be perceived as providing a conclusion to the topic of CA simulation. However, this is not the case, as CAs do more than just running any algorithm. They run distributed algorithms in a distributed manner, model phenomena together with their spatial structure, and allow the use of the spatial parallelism inherent in the model. These features, modelled by CA and not by TM, are all interesting, and so the concepts of simulation and universality needed be revisited in this context to account for space. This has been done by returning to the original meaning of the word *simulation* [1, 7, 11], namely the ability for one instance of a computational model to simulate other instances of the *same* computational model. The introduction of a partial order on CA via groupings [24], and subsequent generalisations [29, 35], have led to elegant and robust definitions of intrinsic simulation. Intrinsic simulation formalises the ability of a CA to simulate another in a space-preserving manner. Intuitively this is exactly what is needed to show the equivalence between the various competing definitions of QCA, *i.e.* that they can all simulate each other in a space-preserving manner. The definition of intrinsic simulation has already been translated in the quantum context [2], however as it stands this is not sufficient to obtain the desired result. In this paper the definition of intrinsic simulation in the quantum context is discussed and developed, before the equivalence between all the various above-mentioned definitions of QCA is tackled.

1.3 QCA: Simplification and Universality

Intrinsic universality is the ability to intrinsically simulate any other QCA. Here we show that the axiomatic style QCA, the multilayer block representation QCA, the two-layer block representation QCA, and the PQCA are equivalent, entailing that PQCA are intrinsically universal. Here the PQCA is chosen as the prime model as it is the simplest way to describe a QCA. Therefore, the result developed in this work is also a simplifying one for the field of QCA as a whole. From a theoretical physics perspective, showing that ‘Partitioned Quantum Cellular

Automata are universal’ is a statement that ‘scattering phenomena are universal physical phenomena’.

There are several related results in the CA literature. Several influential works by Morita *et al* emphasise Reversible Partitioned CA universality. For instance, they provide computation universal Reversible Partitioned CA constructions [26, 27], and their ability to simulate any CA in the one-dimensional case is also shown [25]. The problem of intrinsically universal Reversible CA (RCA) constructions was tackled by Durand-Lose [12, 13]. The difficulty is in having an n -dimensional RCA simulate all other n -dimensional RCA and not, say, the $(n - 1)$ -dimensional RCA, otherwise a history-keeping dimension could be used, as in Toffoli [36]. Strongly related to this is the work on block representations of RCA by Kari [19].

The QCA-related results are focused on universality. Watrous [41] proved that QCA are universal in the sense of QTM. Shepherd, Franz and Werner [34] defined a class of QCA where the scattering unitary U_i changes at each step i (classical control QCA). Universality in the circuit-sense has already been achieved by Van Dam [37], Cirac and Vollbrecht [38], Nagaj and Wocjan [28], and Raussendorf [32]. In the bounded-size configurations case, circuit universality coincides with intrinsic universality, as noted by Van Dam [37]. Intrinsically universal QCA in the one-dimensional case have also been resolved [2]. Finally, a subsequent work, which crucially builds upon the result of this paper, exhibits an n -dimensional intrinsically universal QCA [3]. Given the crucial role of this in classical CA theory [14], the issue of intrinsic universality in the n -dimensional case needed to be addressed. Having then shown that PQCA, a simple subclass of QCA, are intrinsically universal, it remained to show that there existed a n -dimensional PQCA capable of simulating all other n -dimensional PQCA for $n > 1$, which we show in this paper.

The necessary theoretical background for understanding QCA, and hence the problems addressed in this paper, is provided in section 2. Intrinsic simulation is discussed and generalised in section 3. In section 4 the various alternative definitions of QCA are shown to be equivalent to the simplest definition, *i.e.* PQCA. Section 5 concludes with a discussion and ideas for future directions.

2 Definitions

2.1 n -Dimensional QCA

This section provides the axiomatic style definitions for n -dimensional QCA. Configurations hold the basic states of an entire array of cells, and hence denote the possible basic states of the entire QCA:

Definition 1 (Finite configurations) *A (finite) configuration c over Σ is a function $c : \mathbb{Z}^n \rightarrow \Sigma$, with $(i_1, \dots, i_n) \mapsto c(i_1, \dots, i_n) = c_{i_1 \dots i_n}$, such that there exists a (possibly empty) finite set I satisfying $(i_1, \dots, i_n) \notin I \Rightarrow c_{i_1 \dots i_n} = q$, where q is a distinguished quiescent state of Σ . The set of all finite configurations over Σ will be denoted \mathcal{C}_{fin}^Σ .*

Since this work relates to QCA rather than CA, the global state of a QCA can be a superposition of these configurations. To construct the separable Hilbert space of superpositions of configurations the set of configurations must be countable. Thus finite, unbounded, configurations are considered. The quiescent state of a CA is analogous to the blank symbol of a Turing machine tape.

Definition 2 (Superpositions of configurations) Let $\mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$ be the Hilbert space of configurations. Each finite configuration c is associated with a unit vector $|c\rangle$, such that the family $(|c\rangle)_{c \in \mathcal{C}_{fin}^\Sigma}$ is an orthonormal basis of $\mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$. A superposition of configurations is then a unit vector in $\mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$.

Definition 3 (Unitarity) A linear operator $G : \mathcal{H}_{\mathcal{C}_{fin}^\Sigma} \rightarrow \mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$ is unitary if and only if $\{G|c\rangle \mid c \in \mathcal{C}_{fin}^\Sigma\}$ is an orthonormal basis of $\mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$.

Definition 4 (Shift-invariance) Consider the shift operation, for $k \in \{1, \dots, n\}$, which takes configuration c to c' where for all (i_1, \dots, i_n) we have $c'_{i_1 \dots i_k \dots i_n} = c_{i_1 \dots i_k + 1 \dots i_n}$. Let $\sigma_k : \mathcal{H}_{\mathcal{C}_{fin}^\Sigma} \rightarrow \mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$ denote its linear extension to a superpositions of configurations. A linear operator $G : \mathcal{H}_{\mathcal{C}_{fin}^\Sigma} \rightarrow \mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$ is said to be shift invariant if and only if $G\sigma_k = \sigma_k G$ for each k .

The following definition captures the causality of the dynamics. Imposing the condition that the state associated to a cell (its reduced density matrix) is a function of the neighbouring cells is equivalent to stating that information propagates at a bounded speed.

Definition 5 (Causality) A linear operator $G : \mathcal{H}_{\mathcal{C}_{fin}^\Sigma} \rightarrow \mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$ is said to be causal if and only if for any $(i_1, \dots, i_n) \in \mathbb{Z}_n$, there exists a function f such that $\rho'|_{\mathcal{N}} = f(\rho|_{\mathcal{N}})$ for all ρ over $\mathcal{H}_{\mathcal{C}_{fin}^\Sigma}$, where:

$\mathcal{N} = \{i_1, i_1 + 1\} \times \dots \times \{i_n, i_n + 1\}$, $\rho|_{\mathcal{N}}$ means the restriction of ρ to the neighbourhood \mathcal{N} in the sense of the partial trace, and $\rho' = G\rho G^\dagger$.

In the classical case, the definition is that the letter to be read in some given cell i at time $t + 1$ depends only on the state of the cells i to $i + 1$ at time t . Transposed to a quantum setting, the above definition is obtained. To know the state of cell number i , only the states of cells i and $i + 1$ before the evolution need be known.

More precisely, this restrictive definition of causality is known in the classical case as a $\frac{1}{2}$ -neighbourhood cellular automaton, because the most natural way to represent such an automaton is to shift the cells by $\frac{1}{2}$ at each step, so that visually the state of a cell depends on the state of the two cells under it. This definition of causality is not restrictive, as by grouping cells into “supercells” any CA with an arbitrary finite neighbourhood \mathcal{N} can be made into a $\frac{1}{2}$ -neighbourhood CA. The same method can be applied to QCA, so this definition of causality holds without loss of generality. However, the f in the above definition does not directly lead to a constructive definition of a cellular automaton, unlike the local transition function in the classical case [5].

This leads to the definition of an n -dimensional QCA.

Definition 6 (QCA) *An n -dimensional quantum cellular automaton (QCA) is an operator $G : \mathcal{H}_{\mathcal{C}_f^\Sigma} \longrightarrow \mathcal{H}_{\mathcal{C}_f^\Sigma}$ which is unitary, shift-invariant and causal.*

Whilst this is clearly the natural, axiomatic definition QCA, clearly stems from an equivalent definition in the literature, phrased in terms of homomorphism of a C^* -algebra [33]. However, it remains a non-constructive definition and in this sense it can be compared to the Curtis-Hedlund [16] definition of CA as the set of continuous, shift-invariant functions. These definitions characterise (Q)CA via the global, composable properties that they must have; but they do not provide an operational, hands-on description of their dynamics. clearly stems from an equivalent definition in the literature, phrased in terms of homomorphism of a C^* -algebra [33]. This work aims at further simplifying those mathematical objects, down to PQCA.

2.2 Multilayer Block Representation

The axiomatic style definition of QCA remains somewhat abstract and mathematical. A central tool and concept in this paper is that of a (multilayer) block representation of QCA. Intuitively, we say that a QCA G admits a block representation when it can be expressed as blocks, *i.e.* local unitaries, composed in space (via the tensor product) and time (via operator composition), thereby forming a finite-depth quantum circuit infinitely repeating across space. The structure theorem given in previous work [5] states that any QCA can in fact be represented in such a way:

Theorem 1 (n -dimensional QCA multilayer block representation)

Let G be an n -dimensional QCA with alphabet Σ . Let E be an isometry from $\mathcal{H}_\Sigma \rightarrow \mathcal{H}_\Sigma \otimes \mathcal{H}_\Sigma$ such that $E|\psi_x\rangle = |q\rangle \otimes |\psi_x\rangle$. This mapping can be trivially extended to whole configurations, yielding a mapping $E : \mathcal{H}_{C_f^\Sigma} \rightarrow \mathcal{H}_{C_f^{\Sigma^2}}$. There then exists an n -dimensional QCA H on alphabet Σ^2 , such that $HE = EG$, and H admits an 2^n -layer block representation. Moreover H is of the form

$$H = (\bigotimes S)(\prod K_x) \quad (1)$$

where:

- (K_x) is a collection of commuting unitary operators all identical up to shift, each localised upon each neighbourhood \mathcal{N}_x ;
- S is the swap gate over $\mathcal{H}_\Sigma \otimes \mathcal{H}_\Sigma$, hence localised upon each node x .

This theorem therefore bridges the gap between the axiomatic style definition of QCA and the operational descriptions of QCA. Again, it should be compared with the Curtis-Hedlund [16] theorem, which shows the equivalence between the axiomatic definition of CA and the more operational, standard definition, with a local function applied synchronously across space. One can argue that the form given in Eqn. 1 is not that simple. A contribution of this paper is to simplify it down to PQCA.

Amongst the operational definitions of QCA listed in section 1, only that of Perez-Delgado and Cheung [31] is not two-layer. They directly state, after some interesting informal arguments, that QCA are of a form similar to that given in Eqn. 1.

In other words, this theorem says that starting from an axiomatic definition of QCA, such as Shumacher and Werner's [33], one can derive a circuit-like structure for n -dimensional QCA, thereby extending their result to n dimensions. It also shows that operational definitions [31] can be given a rigorous axiomatics. It follows that the definitions of Pérez-Delgado and Cheung [31] and Shumacher and Werner [33] are actually equivalent, up to ancillary cells.

Therefore the axiomatic definition of QCA given in section 2.1 is equivalent to a multilayer block representation. There are, however, several other definitions of QCA, *i.e.* two-layer block representations and PQCA. The aim is to now show that all definitions of QCA can be reconciled via intrinsic simulation. A quantum version of intrinsic simulation has already been developed [2], but only for one-dimensional QCA, and it is not general enough to state the required equivalence. This difficulty is addressed in the next section, where a new concept of intrinsic simulation for n -dimensional QCA is developed with the required properties.

3 Intrinsic Simulation of n -Dimensional QCA

Intrinsic simulation of one CA by another was discussed informally in section 1.2. A pedagogical discussion in the classical case was given by Ollinger [29], and quantised intrinsic simulation has been formalised in the one-dimensional case [2]. This definition is extended to n -dimensions (and relaxed, see details below) here. The potential use of this concept in theoretical physics is also discussed.

Intuitively, ' G simulates H ' is shown by translating the contents of each cell of H into cells of G , running G , and then reversing the translation; this three step process amounts to running H . This translation should be simple (it should not provide a "hidden" way to compute G), should preserve the topology (each cell of H is encoded into cells of G in a way which preserves neighbours), and should be faithful (no information should be lost in translation). This latter requirement relates to the *isometry* property of quantum theory, *i.e.* an inner product preserving evolution with $Enc^\dagger Enc = \mathbb{I}$. This same requirement agrees with the translation being a physical process. The following definitions are thus derived.

Definition 7 (Isometric coding) Consider Σ_G and Σ_H , two alphabets with distinguished quiescent states q_G and q_H , and such that $|\Sigma_H| \leq |\Sigma_G|$. Consider \mathcal{H}_{Σ_G} and \mathcal{H}_{Σ_H} the Hilbert spaces having these alphabets as their basis, and $\mathcal{H}_{\mathcal{C}_{fin}^G}$, $\mathcal{H}_{\mathcal{C}_{fin}^H}$ the Hilbert spaces of finite configurations over these alphabets. Let E be an isometric linear map from \mathcal{H}_{Σ_H} to \mathcal{H}_{Σ_G} which preserves quiescence, *i.e.* such that $E|q_H\rangle = |q_G\rangle$. It trivially extends into an isometric linear map $Enc = (\bigotimes_{\mathbb{Z}^n} E)$ from $\mathcal{H}_{\mathcal{C}_{fin}^H}$ into $\mathcal{H}_{\mathcal{C}_{fin}^G}$, which we call an isometric encoding. Let D be an isometric linear map from \mathcal{H}_{Σ_G} to $\mathcal{H}_{\Sigma_H} \otimes \mathcal{H}_{\Sigma_G}$ which also preserves

quiescence, in the sense that $D|q_G\rangle = |q_H\rangle \otimes |q_G\rangle$. It trivially extends into an isometric linear map $Dec = (\bigotimes_{\mathbb{Z}^n} D)$ from $\mathcal{H}_{\mathcal{C}_{fin}^G}$ into $\mathcal{H}_{\mathcal{C}_{fin}^H} \otimes \mathcal{H}_{\mathcal{C}_{fin}^G}$, which we call an isometric decoding.

The isometries E and D define an isometric coding if the following condition is satisfied:

$$\forall |\psi\rangle \in \mathcal{H}_{\mathcal{C}_{fin}^H}, \exists |\phi\rangle \in \mathcal{H}_{\mathcal{C}_{fin}^G} \quad / \quad |\psi\rangle \otimes |\phi\rangle = Dec(Enc|\psi\rangle).$$

(Here Dec is understood to morally be an inverse function of Enc , but some garbage $|\phi\rangle$ may be omitted.)

Definition 8 (Direct simulation) Consider Σ_G and Σ_H , two alphabets with distinguished quiescent states q_G and q_H , and two QCA G and H over these alphabets. We say that G directly simulates H , if and only if there exists an isometric coding such that

$$\forall i \in \mathbb{N}, \forall |\psi\rangle \in \mathcal{H}_{\mathcal{C}_{fin}^H}, \exists |\phi\rangle \in \mathcal{H}_{\mathcal{C}_{fin}^G} \quad / \quad (G^i|\psi\rangle) \otimes |\phi\rangle = Dec(H^i(Enc|\psi\rangle)).$$

Unfortunately this is not enough for intrinsic simulation, as it implies that $|\Sigma_H| = |\Sigma_G|$. It is often desirable that G simulates H even though the translation:

- takes several cells of H into several cells of G ;
- demands several steps of G in order to simulate several steps of H .

Hence the grouping of cells is required.

Definition 9 (Grouping) Let G be an n -dimensional QCA over alphabet Σ . Let s and t be two integers, q' a word in $\Sigma' = \Sigma^{s^n}$. Consider the iterate global evolution G^t up to a grouping of each hypercube of s^n adjacent cells into one supercell. If this operator can be considered to be a QCA G' over Σ' with quiescent symbol q' , then we say that G' is an (s, t, q') -grouping of G .

A natural way to continue would be to define an intrinsically universal QCA. However, due to the continuity of \mathcal{H} , this approximation can only be up to ϵ . In the companion paper to this we provide a intrinsically universal instance of a QCA with a bound on the finite error [4].

Definition 10 (Intrinsic simulation) Consider Σ_G and Σ_H , two alphabets with distinguished quiescent states q_G and q_H , and two QCA G and H over these alphabets. We say that G intrinsically simulates H if and only if there exists G' , some grouping of G , and H' , some grouping of H , such that G' directly simulates H' .

In other words, G intrinsically simulates H if and only if there exists some isometry E which translates supercells of H into supercells of G , such that if G is iterated and then translated back, the whole process is equivalent to an iteration of H . This understanding is shown schematically in Fig. 1.

Compared with previous work [2], the concept of intrinsic simulation has been modified to allow the grouping in Fig. 1 on the simulated QCA side, and this variation is important to Thm. 2. This is analogous to the classical case [35].

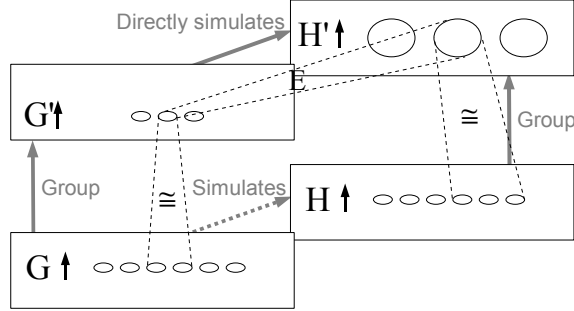


Fig. 1. The concept of intrinsic simulation made formal.

A natural way to follow would be to define the notion of an intrinsically universal QCA. However due to the continuous nature of the underlying Hilbert spaces, no QCA can be intrinsically universal in an exact sense. We can only hope to have a ‘dense’ QCA, *i.e.* one which can simulate any other up to some precision ϵ , which can then be made arbitrarily small. In [3], such an n -dimensional intrinsically universal QCA construction is indeed provided, together with bounds on ϵ . Notice that the latter result [3] crucially relies upon the fact that PQCA are intrinsically universal.

4 Constructions

Now that an appropriate notion of intrinsic simulation has been developed, the problem of showing an equivalence between the different operational definitions of QCA is addressed here.

4.1 Down to Two Layers: Block QCA

Quantisations of block representations of CA are generally presented as two-layer; *cf.* [9, 18, 28, 32, 33, 37]. This is captured by the definition of a Block QCA (BQCA), where $\mathcal{H}^{\otimes 2^n}$ is $\mathcal{H} \otimes \dots \otimes \mathcal{H}$, repeated 2^n times:

Definition 11 (BQCA) *A block n -dimensional quantum cellular automaton (BQCA) is defined by two unitary operators U_0 and U_1 such that $U_i : \mathcal{H}_\Sigma^{\otimes 2^n} \rightarrow \mathcal{H}_\Sigma^{\otimes 2^n}$, and $U_i |qq \dots qq\rangle = |qq \dots qq\rangle$, *i.e.* each takes 2^n cells into 2^n cells and preserves quiescence. Consider $G_i = (\bigotimes_{2\mathbb{Z}^n} U_i)$ the operator over \mathcal{H} . The induced global evolution is G_0 at odd time steps, and σG_1 at even time steps, where σ is a translation by one in all directions (Fig. 2).*

Showing the equivalence of the QCA and BQCA axiomatics is not trivial. In one direction this is simple, as BQCA are unitary, causal, and shift-invariant, and hence fall under the axiomatics and Thm. 1 (strictly speaking we need to

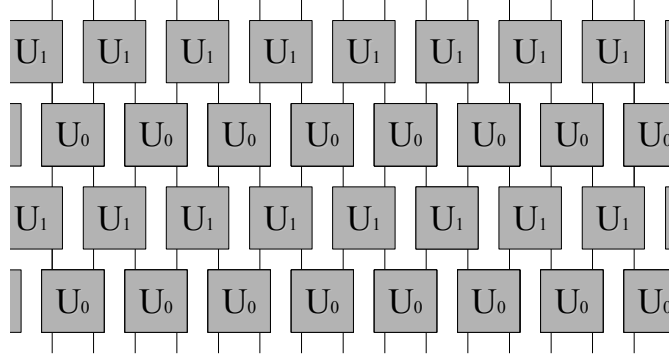


Fig. 2. BQCA. The elementary unitary evolutions U_0 and U_1 are alternated repeatedly as shown, in 1D.

group each hypercube of 2^n adjacent cells into a supercell, see Def. 9.) However, there are several factors to consider regarding the ability of BQCA to simulate any QCA, which are now addressed.

In the form given by Thm. 1, each cell x at time t is successively involved in 2^n computations governed by a local unitary K , whose aim is to compute the next state of a cell within a radius $\frac{1}{2}$ from x at time $t + 1$. In two dimensions, a cell x uses the cells West, North-West and North to work out its North-West successor, and then the cells North, North-East, East of it to compute the North-East successor (Similarly for the South-East and the South-West successors). To mimic this with a BQCA, each original cell can be encoded into four cells, arranged so that the original cell x starts in the North-West quadrant of the four cells. The first layer of the BQCA applies the local unitary K to compute the North-West successor of x . The second layer of the BQCA moves the original cell x in the North-West quadrant. Each full application of the evolution of the BQCA corresponds only to one layer ($\otimes K$), hence it will take four steps for this BQCA to simulate one step of the QCA. Fig. 3 shows a sketch of the method used.

There are some considerations to be discussed. When cell x is turning clockwise in the example, the cell to its North is turning anticlockwise. Hence we need some ancillary data coding for the path to be taken by the original cell x within the four coding cells. Also, Thm. 1 finishes with a *Swap* between the ‘computed tape’, where the results have been stored, and the ‘uncomputed tape’, (*i.e.* what remains of the original cell after having computed all of its successors) which is not shown in the sketch. Hence the number of layers of K computed so far has to be tracked, so that the *Swap* occurs at the appropriate step. The *Swap* also needs to know where the results have been stored in order to move them correctly. All of this has to be arranged spatially and efficiently, and one such method is shown in Figs. 4 and 5.

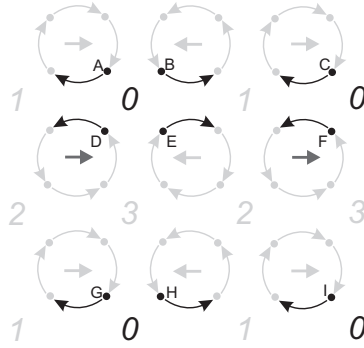


Fig. 3. Sketch of a BQCA simulating a QCA. The original cell x is coded into four cells, at the centre (E). It starts by considering the North-West as at time 0 it will compute its North-West successor, and then move clockwise. At time 1 it will compute its North-East successor, etc.

BQCA can therefore simulate QCA up to a relatively simple encoding, using blocks of four cells. This explains the need for grouping on the simulated QCA side in the revised quantised intrinsic simulation, as in Fig. 1. Encoding groups of cells rather than individual cells is also required for the PQCA discussion (*vide infra*). This encoding is given for two dimensions, but the construct clearly generalises to n -dimensions. Hence QCA (Def. 6) provide a rigorous axiomatics for BQCA (Def. 11), and BQCA provide a convenient operational description of QCA. We have shown that:

Claim 1 (BQCA are universal) *Given any n -dimensional QCA H , there exists an n -dimensional BQCA G which simulates H .*

4.2 Down to One Scattering Unitary: PQCA

Quantisations of partitioned representations of CA are given in several works [17, 37, 41]. These constitute the simplest approach to defining QCA. It is therefore interesting to consider whether QCA (as in Def. 6) provide a rigorous axiomatics for PQCA, and if PQCA provide a convenient operational description of QCA. A PQCA is essentially a BQCA where the two layers apply the same unitary operation, shifted appropriately.

Definition 12 (PQCA) *A partitioned n -dimensional quantum cellular automaton (PQCA) is defined by a scattering unitary operator U such that $U : \mathcal{H}_\Sigma^{\otimes 2^n} \rightarrow \mathcal{H}_\Sigma^{\otimes 2^n}$, and $U |qq \dots qq\rangle = |qq \dots qq\rangle$, i.e. that takes a hypercube of 2^n cells into a hypercube of 2^n cells and preserve quiescence. Consider $G = (\bigotimes_{2\mathbb{Z}^n} U)$, the operator over \mathcal{H} . The induced global evolution is G at odd time steps, and σG at even time steps, where σ is a translation by one in all directions (Fig. 6).*

Following previous results (section 4.1), it is only necessary to show that PQCA can simulate BQCA. Both PQCA and BQCA are two-layer; the only

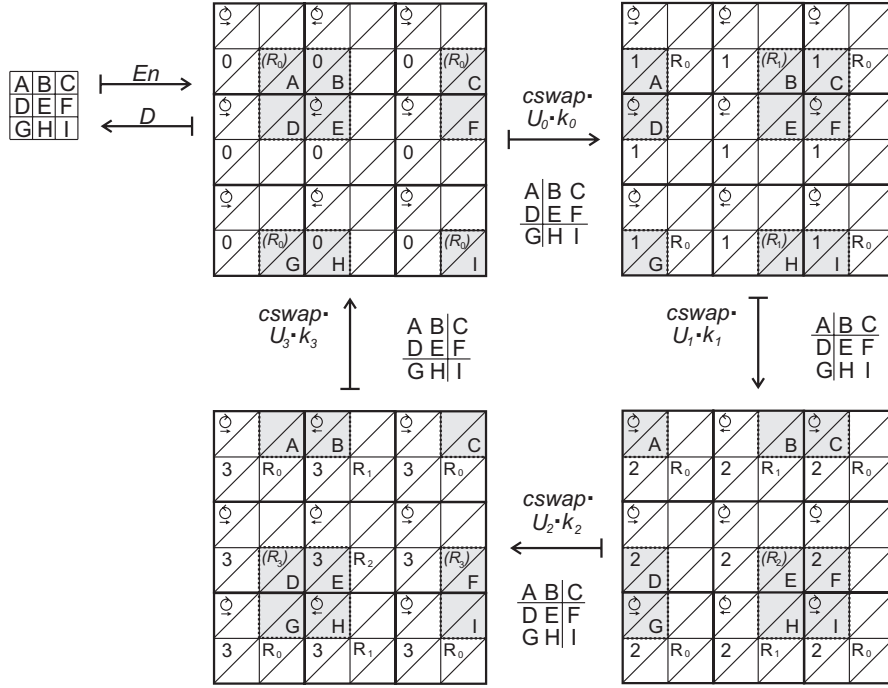


Fig. 4. BQCA simulating a QCA. The grey areas denote the neighbourhood where the action of k_x , the first layer of the BQCA, will be significant – *i.e.* a group of four cells where it will perform a K_x operation to work out a successor. Where this successor will be stored is indicated by (R_x) . At the next step R_x has appeared, and the registers have been reshuffled due to the second layer of the BQCA, which acts according to the rotation-direction mark. The second layer also increases the clock count and includes the final swapping step, which only happens at time 3. There it ensures that R_0 becomes A , R_1 becomes B , etc. Which registers are to be swapped with one another can be calculated from the rotation and arrow marks. Each step is made formal by Fig. 5.

difference is that for BQCA those two layers may be different (*e.g.* compare Figs. 6 and 2), whereas for PQCA there is only a single scattering unitary. So a U -defined PQCA, with a U capable of performing U_0 and U_1 alternatively as controlled by some ancillary suffices. This has been shown for one dimension [2] and is given here for two dimensions in Fig. 7. It is clear that the construct given here generalises to n -dimensions.

Claim 2 (PQCA are universal) *Given any n -dimensional QCA H , there exists an n -dimensional PQCA G which simulates H .*

It can therefore be concluded that PQCA are the most canonical and general operational description of QCA. More generally, by showing here that the various

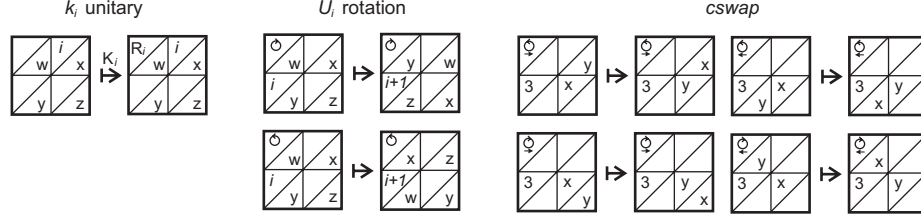


Fig. 5. Operations used in Fig. 4. k applies a K operation whenever some data is present (data carries an extra bit to distinguish it from $|q\rangle$, say). The U operation reshuffles the data by rotating it in the direction given by the indicator in the top left (clockwise or anticlockwise), and increments the index counter. Finally, $cswap$ acts as the identity in all cases except when the index is 3, when it swaps the result of the computations with the data, ready for the next round.

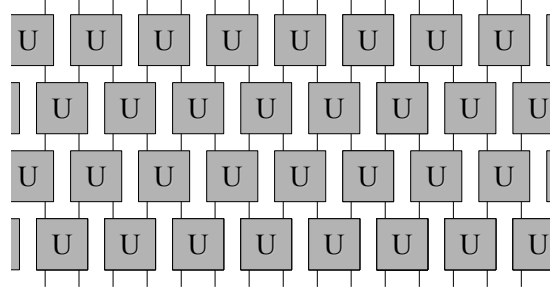


Fig. 6. Partitioned one-dimensional QCA with scattering unitary U . Each line represents a quantum system, in this case a whole cell. Each square represents a scattering unitary U which is applied to two cells. Time flows upwards.

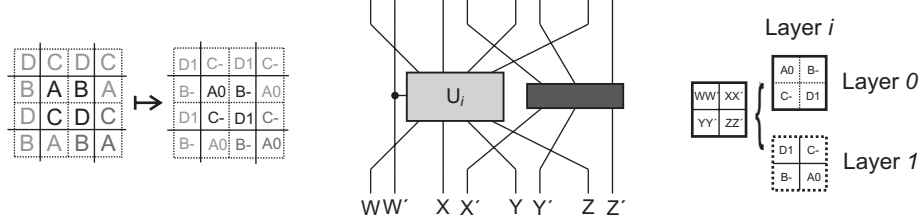


Fig. 7. PQCA simulating a BQCA. The QCA is decorated with control qubits following a simple encoding procedure (*left*), which allow the scattering unitary U (*centre*) to act as either U_0 or U_1 , according to the layer (*right*). The black box can be any unitary.

definitions of QCA available [40, 37, 9, 28, 32, 18, 17, 31] are equivalent, we argue that a well-axiomatised, concrete, and operational n -dimensional QCA is now available.

5 Conclusion

The main contribution of this paper is to show that PQCA are intrinsically universal. There are several consequences, summarised here:

- The construction shows that all the non-axiomatic definitions of QCA [9, 17, 18, 28, 31, 32, 37, 41] are equivalent to one another and to the axiomatic definition, *i.e.* they all simulate each other. Therefore the concept of n -dimensional QCA is well-axiomatised, concrete, and operational.
- The QCA model is simplified, *i.e.* without loss of generality a QCA can be assumed to be a PQCA (see Def. 12).
- The identification of an $n > 1$ -dimensional intrinsically universal QCA is greatly simplified, as it suffices to isolate one $n > 1$ -dimensional PQCA capable of simulating any other n -dimensional PQCA. This is achieved in a subsequent work [3].

Another contribution of this paper is to define and promote n -dimensional intrinsic universality as a useful concept, *per se*. This has to be evaluated within a wider context, explained below.

Universality: From Theoretical Computer Science to Theoretical Physics.

The study of QC has so far aimed to address the issues related to the physical nature of computing, and over the last twenty years there have been a number of quantisations of the classical models of computation, and novel results on the complexity of the tasks that can be encoded in these models. It could be said that theoretical physics has aided theoretical computer science via this path. It is, however, not unlikely that the reverse path could also be productive. This would be part of a bigger trend where theoretical physics departs from looking at ‘matter’ (particles interacting, scattering, forces, etc.) and seeks to look at ‘information’ (entropy, observation, information exchanges between systems, etc.), in an attempt to clarify its own concepts. An example of this is the huge impact that quantum information theory has had on the understanding of foundational concepts such as entanglement [10] and decoherence [30]. A computer science based approach could help to understand basic physical principles, not only in terms of ‘information’, but also in terms of the ‘dynamics of information’, *i.e.* information processing.

Universality, among the many concepts in computer science, is a simplifying methodology in this respect. For example, if the problem being studied crucially involves some idea of interaction, universality makes it possible to cast it in terms of information exchanges *together* with some universal information processing. This paper presents an attempt to export universality as a tool for application in theoretical physics; and hence is a small step towards the goal of finding and understanding what is a *universal physical phenomenon*, within some simplified mechanics. Let us refine this idea:

- Firstly, we want to be able to simulate each physical object independently in its own space. Hence a universal physical phenomenon should be some

elementary unit of computation that can be combined to form a 3D network, accounting for space and interactions across space satisfactorily. (The classical universal TM, on the other hand, does not simulate objects in their own space.)

- Secondly, we want to be able to simulate simple physical objects in an efficient manner, even if they are quantum. Hence a universal physical phenomenon should be a universal model of *quantum* computation. (The classical universal TM is slow at simulating simple quantum phenomena, which suggests that it is not rich enough).

The work that has been presented in this paper formalises an idea of universality which fits both these criteria, namely intrinsic universality over QCA.

A Physical Interpretation.

With this understanding, the intrinsic universality of PQCA developed here could be given a physical interpretation. QCA, as seen through their axiomatic definition (Def. 6), are synonymous with discrete-time, discrete-space quantum mechanics (together with some extra assumptions such as translation-invariance and finite-density of information). Stating that discrete-time, discrete-space quantum mechanical evolutions can, without loss of generality, be assumed to be of the form illustrated in Fig. 6, amounts to the statement that ‘scattering phenomena are universal physical phenomena’. In this sense, the result leads to an understanding of the links between the axiomatic, top-down principles approach to theoretical physics, and the more bottom-up study of the scattering of particles.

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